Momentum Integrators

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Abstract

A discrete total variation calculus with variable time steps is presented in this letter. Using this discrete variation calculus, we generalize Lee's discrete mechanics and derive variational symplectic-energy-momentum integrators by Kane, Marsden and Ortiz. The relationship among discrete total variation, Lee's discrete mechanics and Kane-Marsden-Ortiz's integrators is explored.

Keywords. Total variation, Discrete mechanics, Symplectic-energy-momentum integrators

1 Introduction

In 1980's, Lee proposed an energy-preserving discrete mechanics with variable time steps by taking (discrete) time as dynamical variable [2, 3, 4]. On the other hand, motivated by the symplectic property of Lagrangian mechanics, a version of discrete Lagrangian mechanics has been devoloped and variational integrators that preserve discrete symplectic two form have been obtained [11, 12, 15, 16, 17]. However, variational integrators obtained in this way have fixed time steps and consequently they are not energy-preserving in general.

Obviously, the energy-preserving discrete mechanics and variational integrator are more preferable since solutions of the Euler-Lagrange equations of conservative continuous systems are not only symplectic but also energy-preserving. In order to attain this goal, some discrete mechanics with discrete energy conservation and symplectic variational integrators are needed to study. Recently, Kane, Marsden and Ortiz have employed appropriate time steps to conserve a defined discrete energy and developed what they called symplectic-energy-momentum preserving variational integrators in [10]. Although their approach is more or less related to Lee's discrete mechanics, but the discrete energy preserving condition is not derived by the variational principle.

The purpose of this letter is to generalize or improve these approaches as well as to explore the relation among discrete total variation, Lee's discrete mechanics and Kane-Marsden-Ortiz's integrators. We will present a discrete total variation calculus with variable time steps and a discrete mechanics that is discretely symplectic, energy preserving and has the correct continuous limit. In fact, this discrete variation calculus and mechanics are a generalization of Lee's discrete mechanics in symplectic-preserving sense and can directly derive the variational symplectic-energy-momentum integrators by Kane, Marsden and Ortiz.

This letter is organized as follows. In the next section, we remind total variation calculus for continuous mechanics. In section 3, we present a discrete total variation calculus with variable time steps and a discrete mechanics, derive Kane-Marsden-Ortiz's integrators and explore the relation among our approach, Lee's discrete mechanics and Kane-Marsden-Ortiz's approach. We finish with some conclusions and remarks in Section 4.

Before ending this section, we recall very briefly the ordinary variational principle in Lagrangian mechanics for later use. Suppose Q denotes the extended configuration space with coordinates (t, q^i) and $Q^{(1)}$ the first prolongation of Q with coordinates $(t, q^i, \dot{q}^i)$ [13]. Here t denotes time and $q^i, i = 1, 2, \cdots, n$ denote the position. Consider a Lagrangian $L : Q^{(1)} \to \mathbb{R}$. The corresponding action functional is

$$S(q^i(t)) = \int_a L(t, q^i(t), \dot{q}^i(t))\, dt, \tag{1.1}$$

where $q^i(t)$ is a C^2 curve in Q.

Hamilton's principle seeks a curve $q^i(t)$ denoted by $\mathcal{C}_a^b$ with endpoints a and b, for which the action functional S is stationary under variations of $q^i(t)$ with fixed endpoints. Let

$$V = \phi^i(t, q)\frac{\partial}{\partial q^i} \tag{1.2}$$

be a vertical vector field on Q. Here $q = (q^1, \cdots, q^n)$. By a vertical vector field we mean a vector field on Q not involving terms of form $\xi(t, q)\frac{\partial}{\partial t}$. Namely, time t does not undergo variation.

Let F^ϵ be the flow of V, i.e., a one-parameter group of transformations on Q: $F^\epsilon(t, q^i) = (\tilde{t}, \tilde{q}^i)$.

$$\tilde{t} = t, \tag{1.3}$$

$$\tilde{q}^i = g^i(\epsilon, t, q), \tag{1.4}$$

where

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} g^i(\epsilon, t, q) = \phi^i(t, q) := \delta q^i(t). \tag{1.5}$$

In other words, the deformation (1.3-1.4) transforms the curve $q^i(t)$ into a family of curves $\tilde{q}^i(\epsilon, \tilde{t})$ in Q denoted by $\mathcal{C}_{\epsilon a}^{\ b}$ which are determined by

$$\tilde{t} = t, \tag{1.6}$$

$$\tilde{q}^i = g^i(\epsilon, t, q(t)). \tag{1.7}$$

Thus, we obtain a (sufficiently small) set of curves $\mathcal{C}_{\epsilon a}^{\ b}$ around $\mathcal{C}_a^b$. Corresponding to this set of curves there are a set of Lagrangian and action functionals

$$S(q^i(t)) \to S(\tilde{q}^i(\epsilon, \tilde{t})) = \int_a^b L(\tilde{q}^i(\epsilon, \tilde{t}), \frac{d}{d\tilde{t}}\tilde{q}^i(\epsilon, \tilde{t}))\, d\tilde{t}. \tag{1.8}$$

Now, we can calculate the variation of S at $q(t)$ as follows

$$\begin{aligned}\delta S &= \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} S(\tilde{q}^i(\epsilon, \tilde{t})) \\ &= \int_a^b \left[\left(\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}\right)\phi^i\right] dt + \left.\frac{\partial L}{\partial \dot{q}^i}\phi^i\right|_a^b.\end{aligned} \tag{1.9}$$

For the fixed endpoints, $\phi^i(a, q(a)) = \phi^i(b, q(b)) = 0$, the requirement of Hamilton's principle, $\delta S = 0$, yields the Euler-Lagrangian equation for $q(t)$

$$\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} = 0. \tag{1.10}$$

If we drop the requirement of $\phi^i(a, q(a)) = \phi^i(b, q(b)) = 0$, we can naturally obtain the Lagrangian one form on $Q^{(1)}$ from the second term in (1.9):

$$\theta_L = \frac{\partial L}{\partial \dot{q}^i} dq^i, \tag{1.11}$$

where dq^i are dual to $\frac{\partial}{\partial q^j}$, $dq^i(\frac{\partial}{\partial q^j}) = \delta^i_j$. Furthermore, it can be proved that the solution of (1.10) preserves the Lagrangian two form

$$\omega_L := d\theta_L. \tag{1.12}$$

$$E(q^i, \dot{q}^i) = \{\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}\}dq^i, \tag{1.13}$$

the nilpotency of d leads to

$$dE(q^i, \dot{q}^i) + \frac{d}{dt}\omega_L = 0. \tag{1.14}$$

Namely, the necessary and sufficient condition for symplectic structure preserving is that the Euler-Lagrange one form is closed [6, 7, 8].

2 Total variation for Lagrangian mechanics

Consider a general vector field on Q

$$V = \xi(t,q)\frac{\partial}{\partial t} + \phi^i(t,q)\frac{\partial}{\partial q^i}, \tag{2.1}$$

Here $q = (q^1, \cdots, q^n)$. Let F^ϵ be the flow of V. The variations of $(t, q^i) \in Q$ are described in such a way

$$(t, q^i) \rightarrow F^\epsilon(t, q^i) = (\tilde{t}, \tilde{q}^i), \tag{2.2}$$

where

$$\tilde{t} = f(\epsilon, t, q), \qquad \tilde{q}^i = g^i(\epsilon, t, q), \tag{2.3}$$

with

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} f(\epsilon, t, q) = \xi(t,q) := \delta t, \qquad \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} g^i(\epsilon, t, q) = \phi^i(t,q) := \delta q^i. \tag{2.4}$$

The deformations (2.3) transform a curve $q^i(t)$ in Q denoted by $\mathcal{C}_a^b$ into a set of curves $\tilde{q}^i(\epsilon, \tilde{t})$ in Q denoted by $\mathcal{C}_{\epsilon\tilde{a}}^{\tilde{b}}$, determined by

$$\tilde{t} = f(\epsilon, t, q(t)), \qquad \tilde{q^i} = g^i(\epsilon, t, q(t)). \tag{2.5}$$

Before calculating the total variation of S, we introduce the first order prolongation of V denoted as $\mathrm{pr}^1 V$

$$\mathrm{pr}^1 V = \xi(t,q)\frac{\partial}{\partial t} + \phi^i(t,q)\frac{\partial}{\partial q^i} + \alpha^i(t,q,\dot{q})\frac{\partial}{\partial \dot{q}^i}, \tag{2.6}$$

where

$$\alpha^i(t,q,\dot{q}) = D_t\phi^i(t,q) - \dot{q}^i D_t\xi(t,q), \tag{2.7}$$

where D_t denotes the total derivative with respect to t. For example

$$D_t\phi^k(t,q^i) = \phi_t^k + \phi_{q^i}^k \dot{q}^i, \quad \phi_t^k = \frac{\partial \phi^k}{\partial t}.$$

For prolongation of vector field and the related formulae, we refer the reader to [13].

$$
\begin{aligned}
\delta S &= \frac{d}{d\epsilon}\bigg|_{\epsilon=0} S(\tilde{q}^i(\epsilon,\tilde{t})) \\
&= \frac{d}{d\epsilon}\bigg|_{\epsilon=0} \int_{\tilde{a}}^{\tilde{b}} L(\tilde{t},\tilde{q}^i(\epsilon,\tilde{t}),\frac{d}{d\tilde{t}}\tilde{q}^i(\epsilon,\tilde{t}))\,d\tilde{t} \\
&= \frac{d}{d\epsilon}\bigg|_{\epsilon=0} \int_{a}^{b} L(\tilde{t},\tilde{q}^i(\epsilon,\tilde{t}),\frac{d}{d\tilde{t}}\tilde{q}^i(\epsilon,\tilde{t}))\frac{d\tilde{t}}{dt}\,dt \qquad (\tilde{t}=f(\epsilon,t,q(t))) \\
&= \int_a^b \frac{d}{d\epsilon}\bigg|_{\epsilon=0} L(\tilde{t},\tilde{q}^i(\epsilon,\tilde{t}),\frac{d}{d\tilde{t}}\tilde{q}^i(\epsilon,\tilde{t}))dt + \int_a^b L(t,q^i(t),\dot{q}^i(t))D_t\xi dt \\
&= \int_a^b \left[\frac{\partial L}{\partial t}\xi + \frac{\partial L}{\partial q^i}\phi^i + \frac{\partial L}{\partial \dot{q}^i}(D_t\phi^i - \dot{q}^i D_t\xi)\right] dt + \int_a^b L\, D_t\xi\, dt \\
&= \int_a^b \left[\left(\frac{\partial L}{\partial t} + \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\dot{q}^i - L\right)\right)\xi + \left(\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}\right)\phi^i\right] dt \\
&\quad + \left[\left(L - \frac{\partial L}{\partial \dot{q}^i}\dot{q}^i\right)\xi + \frac{\partial L}{\partial \dot{q}^i}\phi^i\right]\bigg|_a^b .
\end{aligned}
\tag{2.8}
$$

Here we have made use of (2.4), (2.6), (2.7) and

$$
\frac{d}{d\epsilon}\bigg|_{\epsilon=0}\frac{d\tilde{t}}{dt} = \frac{d}{dt}\frac{d}{d\epsilon}\bigg|_{\epsilon=0}\tilde{t} = D_t\xi.
$$

If $\xi(a,q(a)) = \xi(b,q(b)) = 0$ and $\phi^i(a,q(a)) = \phi^i(b,q(b)) = 0$, the requirement of $\delta S = 0$ yields the equation from ξ, the variation along the base manifold, i.e. the time,

$$
\frac{\partial L}{\partial t} + \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\dot{q}^i - L\right) = 0, \tag{2.9}
$$

and the Euler-Lagrange equation from ϕ^i, the variation along the fibre, i.e. the configuration space,

$$
\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} = 0. \tag{2.10}
$$

Here ξ and ϕ^i are regarded as independent components of the total variation. However, there is another decomposition for the independent components, i.e. the vertical and horizontal variations, see *Remark* 2 below.

If L does not depend on t explicitly, i.e., L is conservative, $\frac{\partial L}{\partial t} = 0$, then (2.9) becomes the energy conservation law

$$
\frac{d}{dt}H = 0, \qquad H := \left(\frac{\partial L}{\partial \dot{q}^i}\dot{q}^i - L\right). \tag{2.11}
$$

We expand the left-hand side of (2.11) and obtain

$$
\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\dot{q}^i - L\right) = -\left(\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}\right)\dot{q}^i. \tag{2.12}
$$

Thus, for a conservative L, energy conservation is a consequence of Euler-Lagrange equation. This agrees with Noether theorem, which states that the characteristic of an infinitesimal symmetry of the action functional S is that of a conservation law for the Euler-Lagrange equation. For a conservative L, $\frac{\partial}{\partial t}$ is an infinitesimal symmetry of the action functional S, and its characteristic is $-\dot{q}^i$. From Noether theorem, there exits a corresponding conservation law in the characteristic form

$$
-\left(\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}\right)\dot{q}^i = 0. \tag{2.13}
$$

$$\xi(a, q(a)) = \xi(b, q(b)) = 0, \qquad \phi^i(a, q(a)) = \phi^i(b, q(b)) = 0, \tag{2.14}$$

we can define the extended Lagrangian one form on $Q^{(1)}$ from the second term in (2.8)

$$\vartheta_L := \left(L - \frac{\partial L}{\partial \dot{q}^i}\dot{q}^i\right) dt + \frac{\partial L}{\partial \dot{q}^i} dq^i. \tag{2.15}$$

Suppose $g^i(t, v_{q^i})$ is a solution of (2.10) depending on the initial condition $v_{q^i} \in Q^{(1)}$. Restricting $\tilde{q}^i(\epsilon, \tilde{t})$ to the solution space of (2.10) and using the same method in [11], it can be proved that the extended symplectic two form is preserved

$$(\mathrm{pr}^1 g^i)^* \Omega_L = \Omega_L, \qquad \Omega_L := d\vartheta_L. \tag{2.16}$$

where $\mathrm{pr}^1 g^i(s, v_{q^i})) = (s, g^i(s, v_{q^i}), \frac{d}{ds} g^i(s, v_{q^i}))$ denotes the first order prolongation of $g^i(s, v_{q^i})$ [13].

Remark 1. If ξ in (2.1) is independent of q, the deformations in (2.3) are called fiber-preserving. In this case, the domain of definition of $\tilde{q}^i(\epsilon, \tilde{t})$ only depends on the deformations (2.3). While in the general case, the domain of definition of $\tilde{q}^i(\epsilon, \tilde{t})$ not only depends on the deformations (2.3) but also on $q^i(t)$.

Remark 2. Using the identity

$$\frac{\partial L}{\partial t} + \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\dot{q}^i - L\right) = -\left(\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}\right)\dot{q}^i, \tag{2.17}$$

the Eq. (2.8) becomes

$$\delta S = \int_a^b \left(\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}\right)(\phi^i - \xi \dot{q}^i) dt + \left[\frac{\partial L}{\partial \dot{q}^i}(\phi^i - \xi \dot{q}^i)\right]\Bigg|_a^b + (L\xi)|_a^b. \tag{2.18}$$

According to (2.4), $\phi^i = \delta q^i$ should be regarded as the total variation of q^i, $\delta q^i = \delta_V q^i + \delta_H q^i$, since the variation of t also induces the variation of q^i denoted as $\delta_H q^i$, the horizontal variation of q^i. Due to $\xi = \delta t$ in (2.4), the horizontal variation of q^i should be $\delta_H q^i = \xi \dot{q}^i$ and consequently $\phi^i - \xi \dot{q}^i$ is interpreted as vertical variation $\delta_V q^i$, i.e. the variation of $q^i(t)$ at the moment t (see, for example [1]). Therefore, the first two terms in (2.18) come from vertical variation $\delta_V q^i$ and the last term comes from horizontal variation δt. The horizontal variation of S with respect to the horizontal variation $\delta_H q^i = \xi \dot{q}^i$ just gives rise to the identity (2.17).

3 Discrete mechanics and variational integrators with variable time steps

In this section, by means of a calculus of discrete total variations we develop a discrete Lagrangian mechanics, which includes the boundary terms in Lee's discrete mechanics that give rise to the discrete version of symplectic preserving. The discrete variation calculus is mainly analog to Lee's idea that (discrete) time is regarded as dynamical variable, i.e. the time steps are variable [2, 3, 4]. And the vertical part of this discrete variation calculus is similar to the one in [10, 11, 12, 15, 16, 17]. Using this calculus for discrete total variations we naturally derive Kane-Marsden-Ortiz's integrators.

We use $Q \times Q$ for the discrete version of the first prolongation for the extended configuration space Q. A point $(t_0, q_0; t_1, q_1) \in Q \times Q$ [1]corresponds to a tangent vector $\frac{q_1 - q_0}{t_1 - t_0}$. A discrete Lagrangian is defined to be $\mathbb{L} : Q \times Q \to \mathbb{R}$ and the corresponding action to be

$$\mathbb{S} = \sum_{k=0}^{N-1} \mathbb{L}(t_k, q_k, t_{k+1}, q_{k+1})(t_{k+1} - t_k). \tag{3.1}$$

[1]In this section q is an abbreviation of $(q^1, q^2, \cdots, q^n)$.

$\Phi : Q \times Q \to Q \times Q$ by

$$\Phi(t_{k-1}, q_{k-1}, t_k, q_k) = (t_k, q_k, t_{k+1}, q_{k+1}). \tag{3.2}$$

Here (t_{k+1}, q_{k+1}) are found from the following discrete Euler-Lagrange equation, i.e. the variational integrator, and the discrete energy conservation law (for conservative L)

$$(t_{k+1} - t_k)D_2\mathbb{L}(t_k, q_k, t_{k+1}, q_{k+1}) + (t_k - t_{k-1})D_4\mathbb{L}(t_{k-1}, q_{k-1}, t_k, q_k) = 0, \tag{3.3}$$

and

$$\begin{aligned}(t_{k+1} - t_k)D_1\mathbb{L}(t_k, q_k, t_{k+1}, q_{k+1}) + D_3\mathbb{L}(t_{k-1}, q_{k-1}, t_k, q_k)(t_k - t_{k-1})\\ - \mathbb{L}(t_k, q_k, t_{k+1}, q_{k+1}) + \mathbb{L}(t_{k-1}, q_{k-1}, t_k, q_k) = 0,\end{aligned} \tag{3.4}$$

for all $k \in \{1, 2, \cdots, N-1\}$. Here D_i denotes the partial derivative of $\mathbb{L}$ with respect to the ith argument. The Eq. (3.3) is the discrete Euler-Lagrange equation. The Eq. (3.4) is the discrete energy conservation law for a conservative $\mathbb{L}$. The integrator (3.3)-(3.4) is just Kane-Marsden-Ortiz's integrator.

Using the discrete flow Φ, the Eqs. (3.3) and (3.4) become respectively

$$(t_{k+1} - t_k)D_2\mathbb{L} \circ \Phi + (t_k - t_{k-1})D_4\mathbb{L} = 0, \tag{3.5}$$

$$((t_{k+1} - t_k)D_1\mathbb{L} - \mathbb{L}) \circ \Phi + D_3\mathbb{L} + \mathbb{L} = 0. \tag{3.6}$$

If $(t_{k+1} - t_k)D_2\mathbb{L}$ and $(t_{k+1} - t_k)D_1\mathbb{L} - \mathbb{L}$ are invertible, the Eqs. (3.5) and (3.6) determine the discrete flow Φ under the consistency condition

$$((t_{k+1} - t_k)D_1\mathbb{L} - \mathbb{L})^{-1} \circ (D_3\mathbb{L} + \mathbb{L}) = ((t_{k+1} - t_k)D_2\mathbb{L})^{-1} \circ (t_k - t_{k-1})D_4\mathbb{L}. \tag{3.7}$$

Now we prove that the discrete flow Φ preserves a discrete version of the extended Lagrange two form Ω_L. As in continuous case, we calculate $d\mathbb{S}$ for variations with varied endpoints.

$$\begin{aligned}
& d\mathbb{S}(t_0, q_0, \cdots, t_N, q_N) \cdot (\delta t_0, \delta q_0, \cdots, \delta t_N, \delta q_N) \\
&= \sum_{k=0}^{N-1} (D_2L(t_k, q_k, t_{k+1}, q_{k+1})\delta q_k + D_4L(t_k, q_k, t_{k+1}, q_{k+1})\delta q_{k+1})(t_{k+1} - t_k) \\
&\quad + \sum_{k=0}^{N-1} (D_1L(t_k, q_k, t_{k+1}, q_{k+1})\delta t_k + D_3L(t_k, q_k, t_{k+1}, q_{k+1})\delta t_{k+1})(t_{k+1} - t_k) \\
&\quad + \sum_{k=0}^{N-1} L(t_k, q_k, t_{k+1}, q_{k+1})(\delta t_{k+1} - \delta t_k) \\
&= \sum_{k=0}^{N-1} D_2L(t_k, q_k, t_{k+1}, q_{k+1})(t_{k+1} - t_k)\delta q_k \\
&\quad + \sum_{k=1}^{N} D_4L(t_{k-1}, q_{k-1}, t_k, q_k)(t_k - t_{k-1})\delta q_k \\
&\quad + \sum_{k=0}^{N-1} D_1L(t_k, q_k, t_{k+1}, q_{k+1})(t_{k+1} - t_k)\delta t_k \\
&\quad + \sum_{k=1}^{N} D_3L(t_{k-1}, q_{k-1}, t_k, q_k)(t_k - t_{k-1})\delta t_k \\
&\quad + \sum_{k=0}^{N-1} L(t_k, q_k, t_{k+1}, q_{k+1})(-\delta t_k) + \sum_{k=1}^{N} L(t_{k-1}, q_{k-1}, t_k, q_k)\delta t_k
\end{aligned}$$

$$
\begin{aligned}
&+\sum_{k=1}^{N-1}(D_1L(t_k,q_k,t_{k+1},q_{k+1})(t_{k+1}-t_k)+D_3L(t_{k-1},q_{k-1},t_k,q_k)(t_k-t_{k-1})\\
&\qquad +L(t_{k-1},q_{k-1},t_k,q_k)-L(t_k,q_k,t_{k+1},q_{k+1}))\delta t_k\\
&+D_2L(t_0,q_0,t_1,q_1)(t_1-t_0)\delta q_0+D_4L(t_{N-1},q_{N-1},t_N,q_N)(t_N-t_{N-1})\delta q_N\\
&+(D_1L(t_0,q_0,t_1,q_1)(t_1-t_0)-L(t_0,q_0,t_1,q_1))\delta t_0\\
&+(D_3L(t_{N-1},q_{N-1},t_N,q_N)(t_N-t_{N-1})+L(t_{N-1},q_{N-1},t_N,q_N))\delta t_N.
\end{aligned}
\tag{3.8}
$$

We can see that the last four terms in (3.8) come from the boundary variations. Based on the boundary variations, we can define two one forms on $Q \times Q$

$$
\begin{aligned}
&\theta_{\mathbb{L}}^{-}(t_k,q_k,t_{k+1},q_{k+1})\\
&=(D_1\mathbb{L}(t_k,q_k,t_{k+1},q_{k+1})(t_{k+1}-t_k)-\mathbb{L}(t_k,q_k,t_{k+1},q_{k+1}))dt_k\\
&\quad +D_2\mathbb{L}(t_k,q_k,t_{k+1},q_{k+1})(t_{k+1}-t_k)dq_k,
\end{aligned}
\tag{3.9}
$$

and

$$
\begin{aligned}
&\theta_{\mathbb{L}}^{+}(t_k,q_k,t_{k+1},q_{k+1})\\
&=(D_3\mathbb{L}(t_k,q_k,t_{k+1},q_{k+1})(t_{k+1}-t_k)+\mathbb{L}(t_k,q_k,t_{k+1},q_{k+1}))dt_{k+1}\\
&\quad +D_4\mathbb{L}(t_k,q_k,t_{k+1},q_{k+1})(t_{k+1}-t_k)dq_{k+1}.
\end{aligned}
\tag{3.10}
$$

Here we have employed the notations in [11]. We regard the pair $(\theta_{\mathbb{L}}^{-},\theta_{\mathbb{L}}^{+})$ as the discrete version of the extended Lagrange one form ϑ_L defined in (2.15).

Now we parameterize the solutions of the discrete variational principle by the initial condition (t_0,q_0,t_1,q_1) and restrict $\mathbb{S}$ to that solution space. Then Eq. (3.8) becomes

$$
\begin{aligned}
&d\mathbb{S}(t_0,q_0,\cdots,t_N,q_N)\cdot(\delta t_0,\delta q_0,\cdots,\delta t_N,\delta q_N)\\
&=\theta_{\mathbb{L}}^{-}(t_0,q_0,t_1,q_1)\cdot(\delta t_0,\delta q_0,\delta t_1,\delta q_1)\\
&\quad +\theta_{\mathbb{L}}^{+}(t_{N-1},q_{N-1},t_N,q_N)\cdot(\delta t_{N-1},\delta q_N,\delta t_{N-1},\delta q_{N-1})\\
&=\theta_{\mathbb{L}}^{-}(t_0,q_0,t_1,q_1)\cdot(\delta t_0,\delta q_0,\delta t_1,\delta q_1)\\
&\quad +(\Phi^{N-1})^{*}\theta_{\mathbb{L}}^{+}(t_0,q_0,t_1,q_1)\cdot(\delta t_0,\delta q_0,\delta t_1,\delta q_1).
\end{aligned}
\tag{3.11}
$$

From (3.11), we can obtain

$$
d\mathbb{S}=\theta_{\mathbb{L}}^{-}+(\Phi^{N-1})^{*}\theta_{\mathbb{L}}^{+}. \tag{3.12}
$$

The Eq. (3.12) holds for arbitrary $N>1$. By taking N=2, it leads to

$$
d\mathbb{S}=\theta_{\mathbb{L}}^{-}+\Phi^{*}\theta_{\mathbb{L}}^{+}. \tag{3.13}
$$

Taking exterior differentiation of (3.13), it follows that

$$
\Phi^{*}(d\theta_{\mathbb{L}}^{+})=-d\theta_{\mathbb{L}}^{-}. \tag{3.14}
$$

From the definition of $\theta_{\mathbb{L}}^{-}$ and $\theta_{\mathbb{L}}^{+}$, we know that

$$
\theta_{\mathbb{L}}^{-}+\theta_{\mathbb{L}}^{+}=d(\mathbb{L}(t_{k+1}-t_k)). \tag{3.15}
$$

Taking exterior differentiation of (3.15), we obtain $d\theta_{\mathbb{L}}^{+}=-d\theta_{\mathbb{L}}^{-}$. Define

$$
\Omega_{\mathbb{L}}\equiv d\theta_{\mathbb{L}}^{+}=-d\theta_{\mathbb{L}}^{-}. \tag{3.16}
$$

$$\Phi^*(\Omega_{\mathbb{L}}) = \Omega_{\mathbb{L}}. \tag{3.17}$$

Now we show that the variational integrator (3.3), the discrete energy conservation law (3.4) and the discrete extended Lagrange two form $\Omega_{\mathbb{L}}$ converge to their continuous counterparts as $t_{k+1} \to t_k,\ t_{k-1} \to t_k$.

Consider a conservative Lagrangian $L(q, \dot{q})$. For simplicity, we choose the discrete Lagrangian as

$$\mathbb{L}(t_k, q_k, t_{k+1}, q_{k+1}) = L(q_k, \frac{q_{k+1} - q_k}{t_{k+1} - t_k}). \tag{3.18}$$

The variational integrator (3.3) becomes

$$\frac{\partial L}{\partial q_k}(q_k, \Delta_t q_k) - \frac{1}{t_{k+1} - t_k}\left(\frac{\partial L}{\partial \Delta_t q_k}(q_k, \Delta_t q_k) - \frac{\partial L}{\partial \Delta_t q_{k-1}}(q_{k-1}, \Delta_t q_{k-1})\right) = 0, \tag{3.19}$$

where $\Delta_t q_k = \frac{q_{k+1} - q_k}{t_{k+1} - t_k}, \quad \Delta_t q_{k-1} = \frac{q_k - q_{k-1}}{t_k - t_{k-1}}$.

It is easy to see that as $t_{k+1} \to t_k,\ t_{k-1} \to t_k$, the Eq. (3.19) converges to

$$\frac{\partial L}{\partial q_k} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_k} = 0. \tag{3.20}$$

The discrete energy conservation law (3.4) becomes

$$\frac{E_{k+1} - E_k}{t_{k+1} - t_k} = 0, \tag{3.21}$$

where

$$\begin{aligned} E_{k+1} &= \frac{\partial L}{\partial \Delta_t q_k}\Delta_t q_k - L(q_k, \frac{q_{k+1} - q_k}{t_{k+1} - t_k}) \\ E_k &= \frac{\partial L}{\partial \Delta_t q_{k-1}}\Delta_t q_{k-1} - L(q_{k-1}, \frac{q_k - q_{k-1}}{t_k - t_{k-1}}). \end{aligned}$$

The Eq. (3.21) converges to

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_k}\dot{q}_k - L\right) = 0 \tag{3.22}$$

as $t_{k+1} \to t_k,\ t_{k-1} \to t_k$.

Now we consider the discrete extended Lagrange two form $\Omega_{\mathbb{L}}$ defined by (3.16). Under the discretization (3.18), the discrete extended Lagrange one form $\theta_{\mathbb{L}}^+$ defined in (3.10) becomes

$$\theta_{\mathbb{L}}^+ = \left(L(q_k, \Delta_t q_k) - \frac{\partial L}{\partial \Delta_t q_k}\Delta_t q_k\right) dt_{k+1} + \frac{\partial L}{\partial \Delta_t q_k} dq_{k+1}. \tag{3.23}$$

From (3.23), we can deduce that $\theta_{\mathbb{L}}^+$ converges to the continuous Lagrangian one form ϑ_L defined by (2.15) as $t_{k+1} \to t_k,\ t_{k-1} \to t_k$. Thus, we obtain

$$\Omega_{\mathbb{L}} = d\theta_{\mathbb{L}}^+ \to d\vartheta_L = \Omega_L, \quad (t_{k+1} \to t_k,\ t_{k-1} \to t_k). \tag{3.24}$$

The variational integrator (3.3) with fixed time steps does not conserve the discrete energy exactly in general but the computed energy will not have secular variation [5, 14]. In some cases such as in discrete mechanics proposed by Lee in [2, 3, 4], the integrator (3.3) is required to conserve the discrete energy (3.4) by varying the time steps. In other words, the time steps can be chosen according to (3.4) so as to the integrator (3.3) conserves the discrete energy (3.4). The resulting integrator also conserves the discrete extended Lagrange two form $d\theta_{\mathbb{L}}^+$. This fact had not been discussed in Lee's discrete mechanics.

We have presented the calculus of total variation problem for discrete mechanics with variable time steps referring the one for continuous mechanics in this letter. Using the calculus for discrete total variations, we have proved that Lee's discrete mechanics is symplectic and derived Kane-Marsden-Ortiz's integrators. It is well acknowledged, an energy-preserving variational integrator is a more preferable and natural candidate of approximations for conservative Euler-Lagrangian equation since the solution of conservative Euler-Lagrangian equation is not only symplectic but also energy-preserving.

As is mentioned, Kane-Marsden-Ortiz's integrators are closely related to the discrete mechanics proposed by Lee [2, 3, 4]. In Lee's discrete mechanics, the difference equations are just Kane-Marsden-Ortiz's integrators. However, Lee's difference equations are solved as boundary value problems, while Kane-Marsden-Ortiz's integrators are solved as initial value problems.

Finally, it should be mentioned that two of the authors (HYG and KW) and their collaborators have presented a difference discrete variational calculus and the discrete version of Euler-Lagrange cohomology for vertical variation problems in both Lagrangian and Hamiltonian formalism for discrete mechanics and field theory very recently [6, 9]. In their approach, the difference operator with fixed step-length is regarded as an entire geometric object. The advantages of this approach have already be seen in the last section in the course of taking continuous limits although the difference operator Δ_t in (3.18) is of variable step-length. This approach should be able to be generalized for the discrete total variation problems.

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